Scalable and Robust Computational Tools for High-End Computing

The DOE Advanced CompuTational Software Collection (ACTS)

Thirteenth
DOE ACTS Collection Workshop
Berkeley, California, August 14-17, 2012

Tony Drummond
Computational Research Division
Lawrence Berkeley National Laboratory

BERKELEY LAB
Lawrence Berkeley National Laboratory

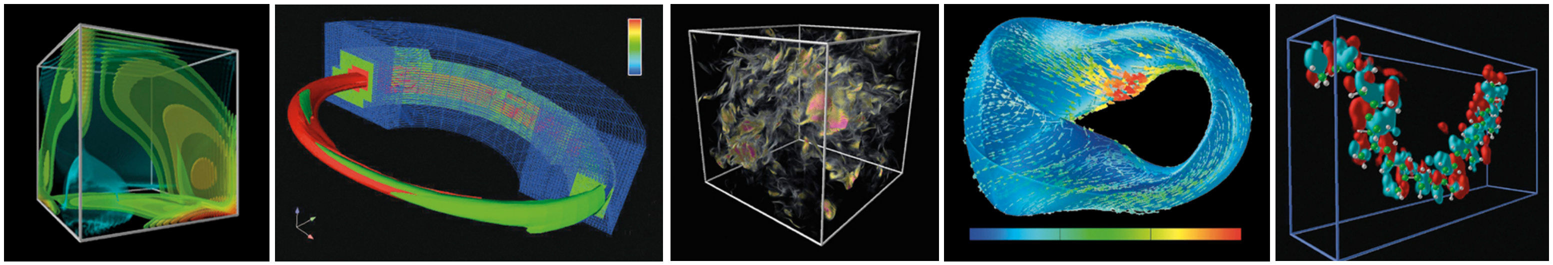
ACTS COLLECTION

U.S. DEPARTMENT OF ENERGY | Office of Science

OUTLINE

- Motivation
- Hardware Trend
- HPC Software Stack
- The DOE ACTS Collection
  - ACTS Functionality
  - Interfaces and Interoperability
- The 12th DOE ACTS Collection Workshop
  - Agenda
- Acknowledgements

The DOE ACTS Collection



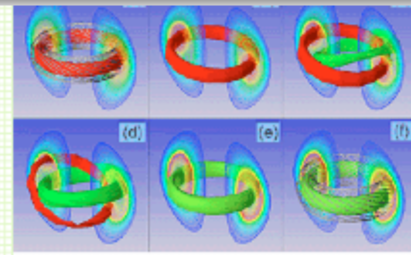
Goal: The Advanced CompuTational Software Collection (ACTS) makes reliable and efficient software tools more widely used, and more effective in solving the nation's engineering and scientific problems.

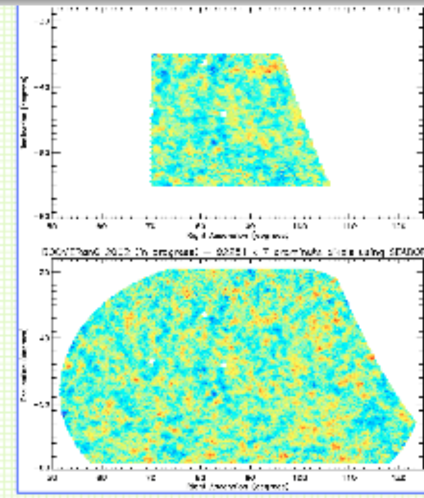
References:

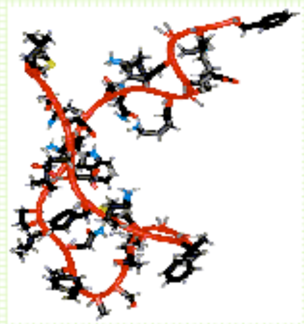
- L.A. Drummond, O. Marques: An Overview of the Advanced CompuTational Software (ACTS) Collection. ACM Transactions on Mathematical Software Vol. 31 pp. 282-301, 2005
- http://acts.nersc.gov

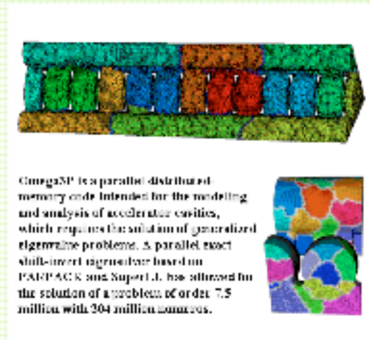
Motivation - HPC Applications

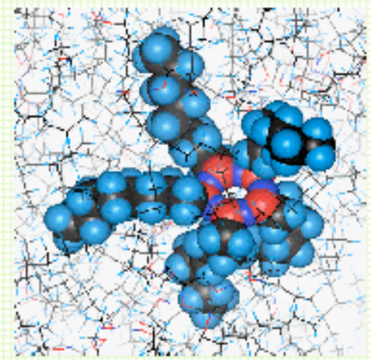
- Accelerator Science
- Astrophysics
- Biology
- Chemistry
- Earth Sciences
- Materials Science
- Nanoscience
- Plasma Science
-
-





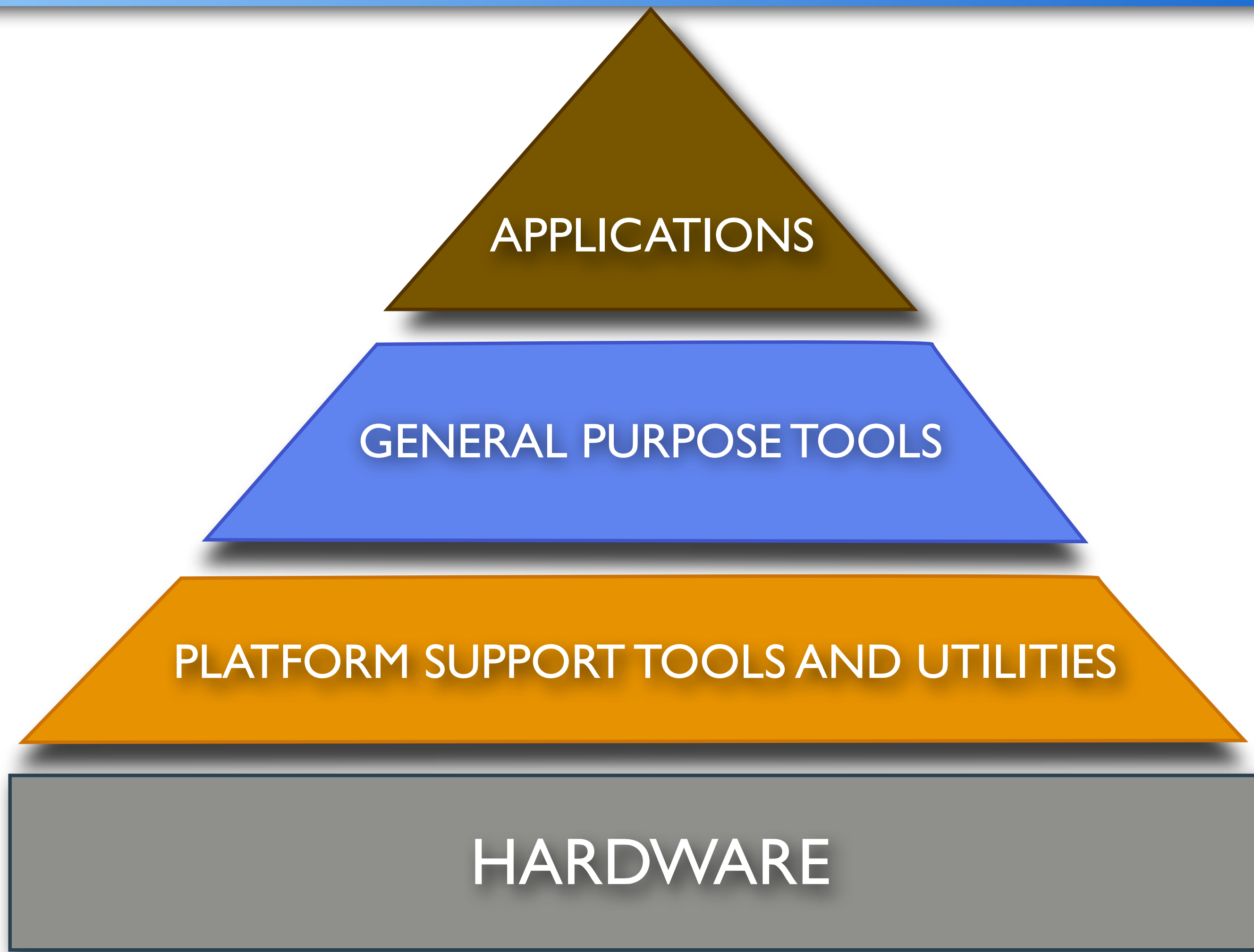




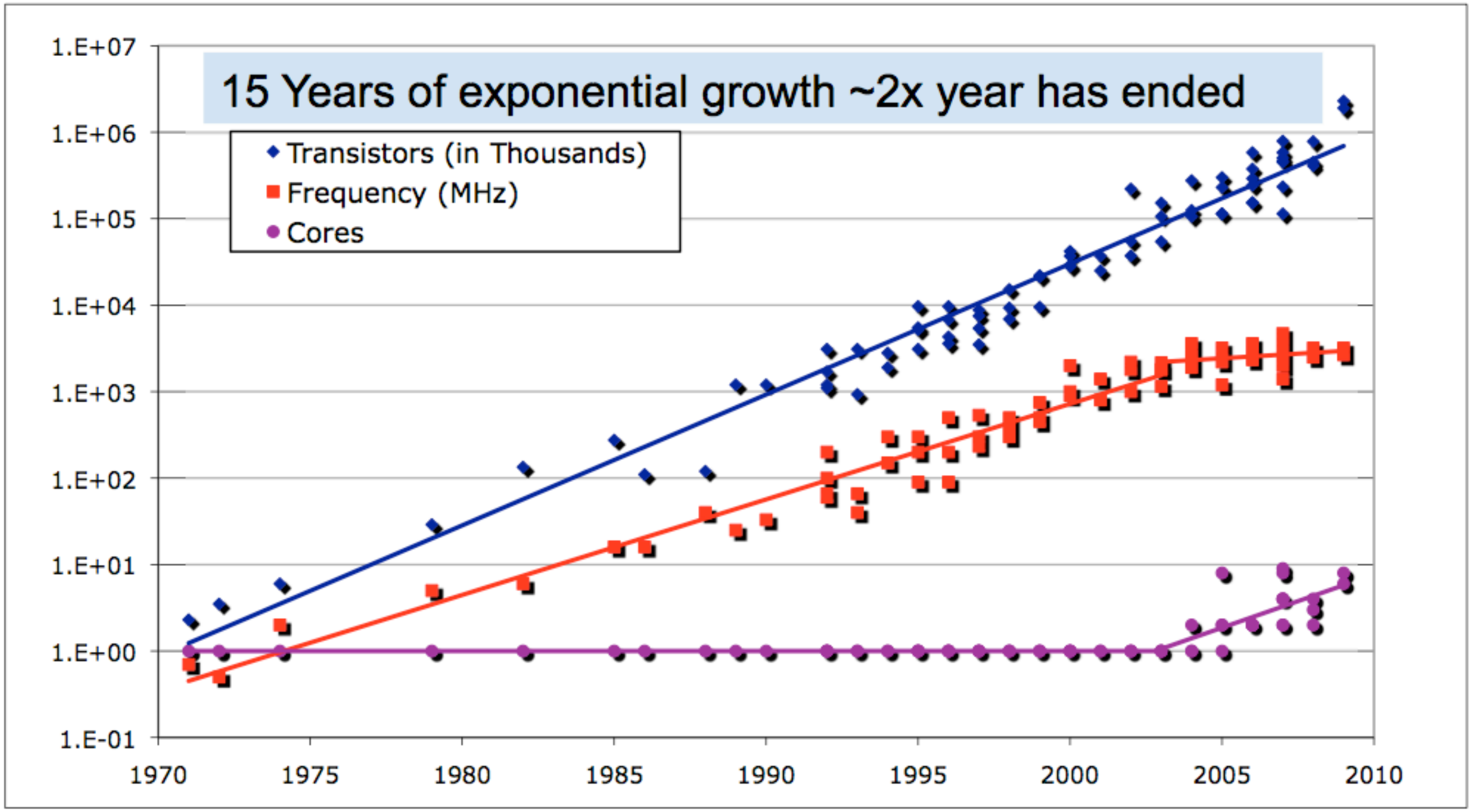


Commonalities:
- Major advancements in Science
- Increasing demands for computational power
- Rely on available computational systems, languages, and software tools

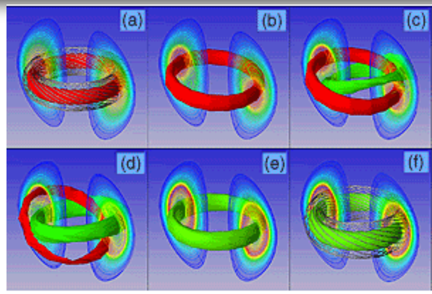
HPC Software Stack

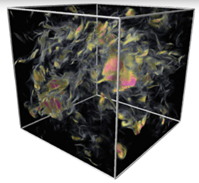


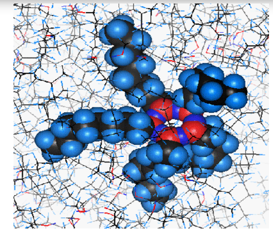
Hardware Trend

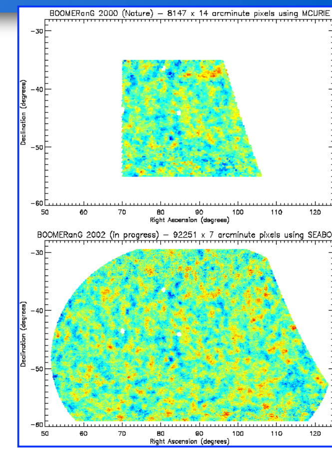


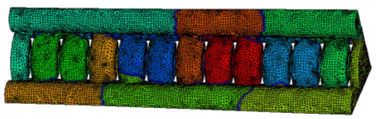
HPC Software Stack











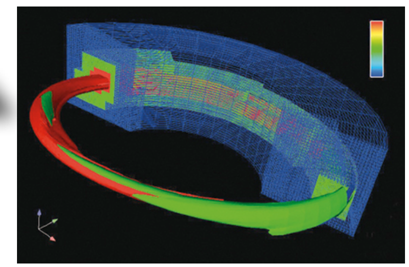
Omega3P is a parallel distributed-memory code intended for the modeling and analysis of accelerator cavities, which requires the solution of generalized eigenvalue problems. A parallel exact shift-invert eigensolver based on PARPACK and SuperLU has allowed for the solution of a problem of order 7.5 million with 304 million nonzeros.

APPLICATIONS

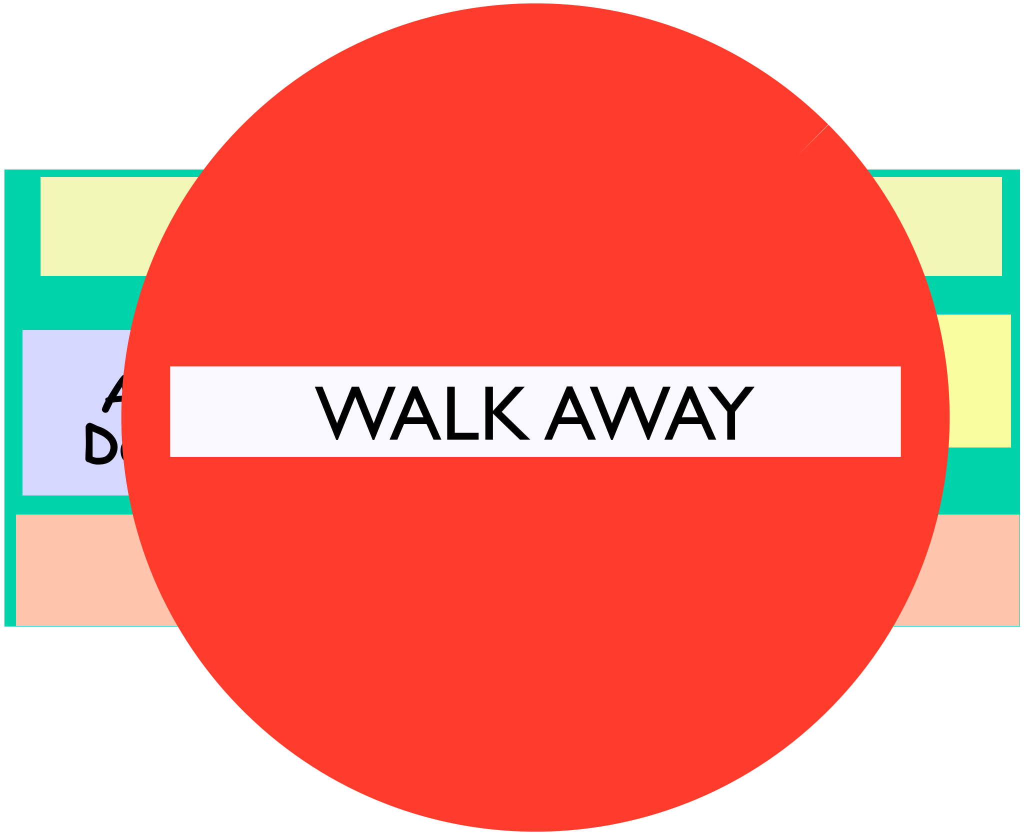
GENERAL PURPOSE TOOLS

PLATFORM SUPPORT TOOLS AND UTILITIES

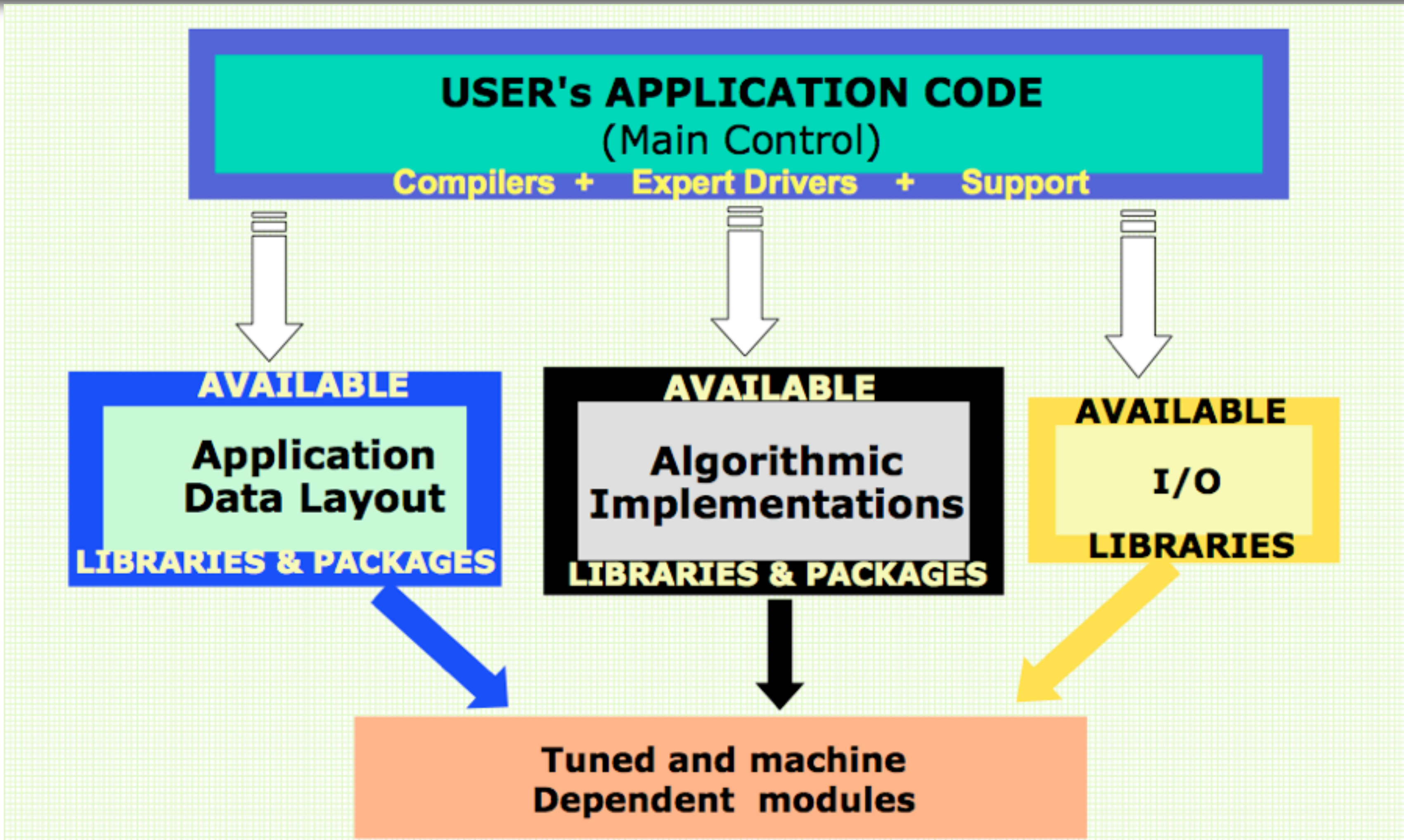
HARDWARE



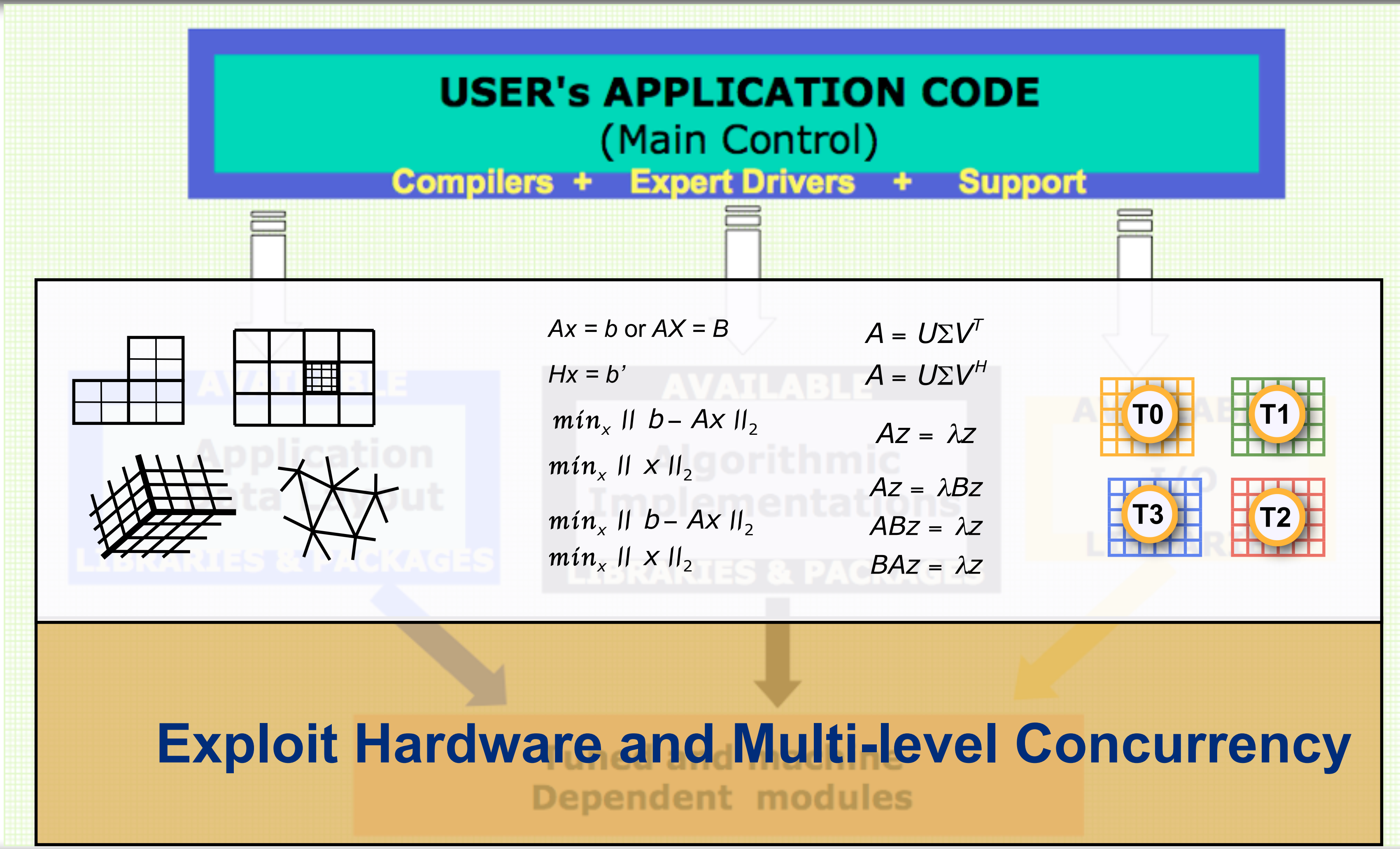
Development of High-End Computing Software



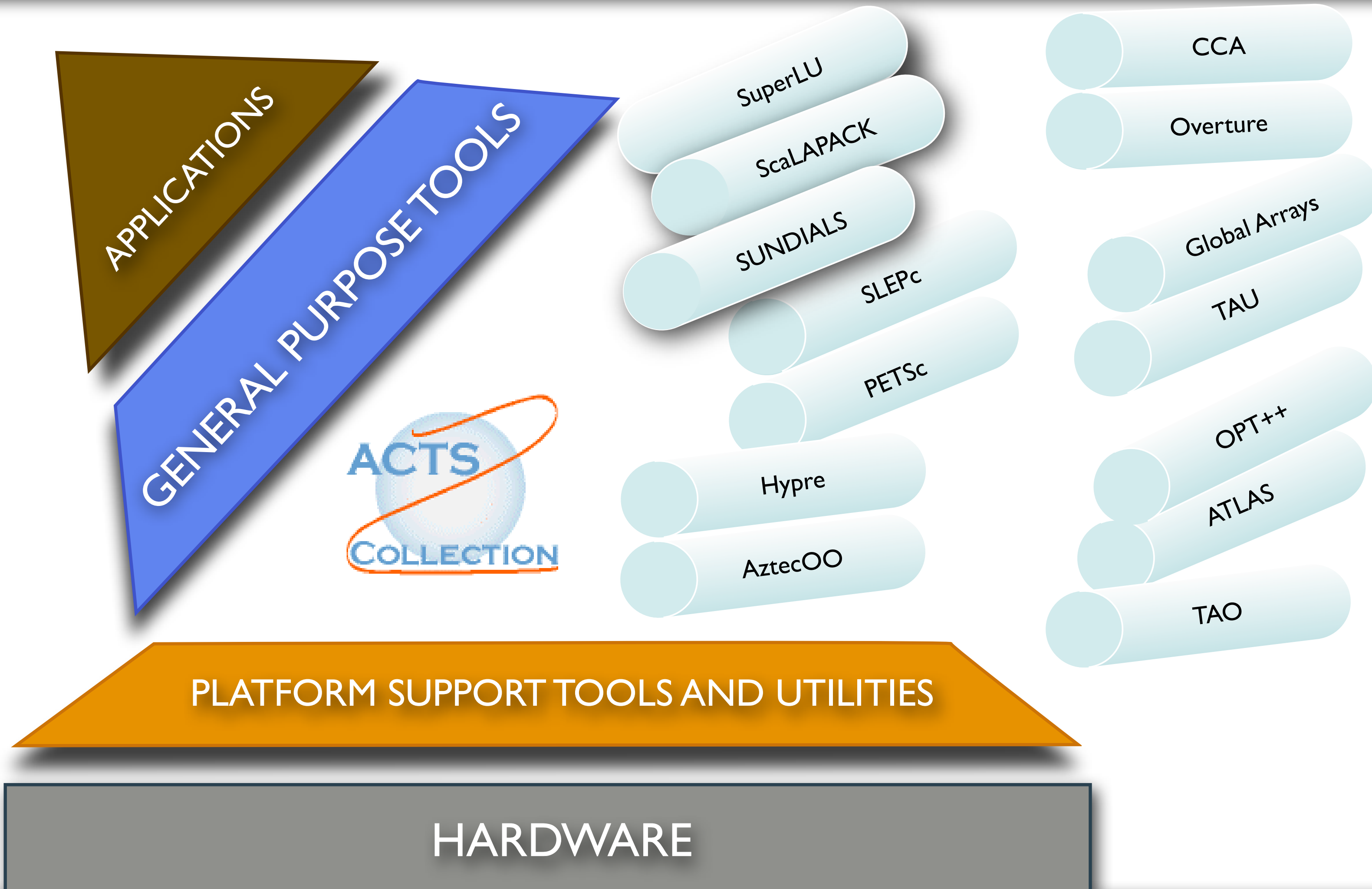
Fast-track The Development of High End Software



Fast-track The Development of High End Software



HPC Software Stack



Current State of DOE ACTS Collection

Category	Tool	Functionalities
Numerical	AztecOO	Scalable linear and non-linear solvers using iterative schemes.
	Hypre	A family of scalable preconditioners.
	PETSc	Scalable linear and non-linear solvers and additional support for PDE related work.
	SUNDIALS	Solvers for the solution of systems of ordinary differential equations, nonlinear algebraic equations, and differential-algebraic equations.
	ScaLAPACK	High performance parallel dense linear algebra.
	SLEPc	Scalable algorithms for the solution of large sparse eigenvalue problems.
	SuperLU	Scalable direct solution of large, sparse, nonsymmetric linear systems of equations.
	TAO	Large-scale optimization software.
Code Development	Global Arrays	Supports the development of parallel programs.
	Overture	Supports the development of computational fluid dynamics codes in complex geometries.
Run Time Support	TAU	Portable and scalable performance analyzes and tracing tools for C, C++, Fortran and Java programs.
Library Development	ATLAS	Automatic generation of optimized numerical dense algebra for scalar processors.

Category	Tool	Functionalities
Tools in Consideration	ML	Multilevel Preconditioners from Trilinos
	BELOS	Krylov based solvers from Trilinos
	Zoltan	Parallel Partitional, Data-Management and Load Balancing
	pOSKI	Sparse auto-tuning library

Considering 4 more

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
What is the computational problem? • numerical (solvers, discretization, meshing, etc. .) • Parallel Programming • Profiling • Debugging at large scale • Programming Model • Auto-Tuning	Available Methods in ACTS	Available algorithms and their HPC implementations in ACTS	Specific ACTS Libraries or Tools that provides that functionality

Solution of Linear Systems

Computational Problem
Systems of Linear Equations $Ax = b$ or $AX = B$

- Solution of systems of linear equations may seem easy, but is at the heart of many computational problems.
- The choice of methods and algorithms to solve these problems depends on matrix characteristics;
  - Symmetric vs nonsymmetric
  - Positive definite vs indefinite
  - Dimension
  - SparsitySpecial structures
    - Banded; block bordered diagonal
    - Conditioning

Solution of Linear Systems

Computational Problem

Systems of Linear Equations

$Ax = b$ or

$AX = B$

Primarily, two flavors of methods:

- DIRECT

  $$\text{compute } A^{-1}$$

  $$x = A^{-1}b$$

- ITERATIVE

  $$\text{compute } \{x^{(0)}, x^{(1)}, \ldots x^{(k)}\}$$

  $$\min |A x^{(k)} - b|$$

- Hybrid
  - preconditioning methods
  - multi-level solvers
    - Algebraic and Geometric Multigrid

Solution of Linear Systems

Computational Problem
Systems of Linear Equations $Ax = b$ or $AX = B$

DIRECT	ITERATIVE
Finite no. of ops	Unknown number of ops. • Convergence depends on A, machine precision, etc. .
Pivoting may be needed to maintain stability	May need preconditioning to improve convergence
Harder to implement	Easier to implement
More communication	Less communication
Large memory requirement	Low Memory requirements
Complex data structure	Simple data structures
More graph problems • Ordering, symbolic manipulation	Fewer graph problems
Easy to handle multiple RHS	Handling of multiple RHS is more difficult

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations $Ax = b$ or $AX = B$	Direct Methods	LU Factorization	ScaLAPACK(dense) SuperLU (sparse)
		Cholesky Factorization	ScaLAPACK
		LDL^T (Tridiagonal matrices)	ScaLAPACK
		QR Factorization	ScaLAPACK
		QR with column pivoting	ScaLAPACK
		LQ factorization	ScaLAPACK

Comparison Between Direct and Iterative Solvers

- Direct methods or iterative methods?
  - Depend on dimensions, sparsity, and conditioning
  - Sparse direct solvers have become very efficient.
    - Almost all sparse direct solvers are built on top of dense matrix operations.
  - Direct methods are desirable when
    - Poor conditioning
    - High accuracies are desired
    - Small dimensions … How small is "small"?
      - Really depend on memory requirement and time to solution
    - Solving multiple linear systems with the same matrix
      - Only one factorization required

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations $Ax = b$ or $AX = B$	Direct Methods	LU Factorization	ScaLAPACK(dense) SuperLU (sparse)
		Cholesky Factorization	ScaLAPACK
		LDL^T (Tridiagonal matrices)	ScaLAPACK
		QR Factorization	ScaLAPACK
		QR with column pivoting	ScaLAPACK
		LQ factorization	ScaLAPACK

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations *(cont..)* $Ax = b$ or $AX = B$	Iterative Methods	Conjugate Gradient	AztecOO (Trilinos) PETSc
		GMRES	AztecOO PETSc Hypre
		CG Squared	AztecOO PETSc
		Bi-CG Stab	AztecOO PETSc
		Quasi-Minimal Residual (QMR)	AztecOO
		Transpose Free QMR	AztecOO PETSc

PETSc's (Develop @ ANL)

Krylov Subspace Methods

GMRES	CG	CGS	Bi-CG-STAB	TFQMR	Richardson	Chebychev	Other

Preconditioners

Additive Schwartz	Block Jacobi	Jacobi	ILU	ICC	LU (Sequential only)	Others

Matrices

Compressed Sparse Row (AIJ)	Blocked Compressed Sparse Row (BAIJ)	Block Diagonal (BDIAG)	Dense	Matrix-free	Other

Distributed Vectors

Index

Indices	Block Indices	Stride	Other

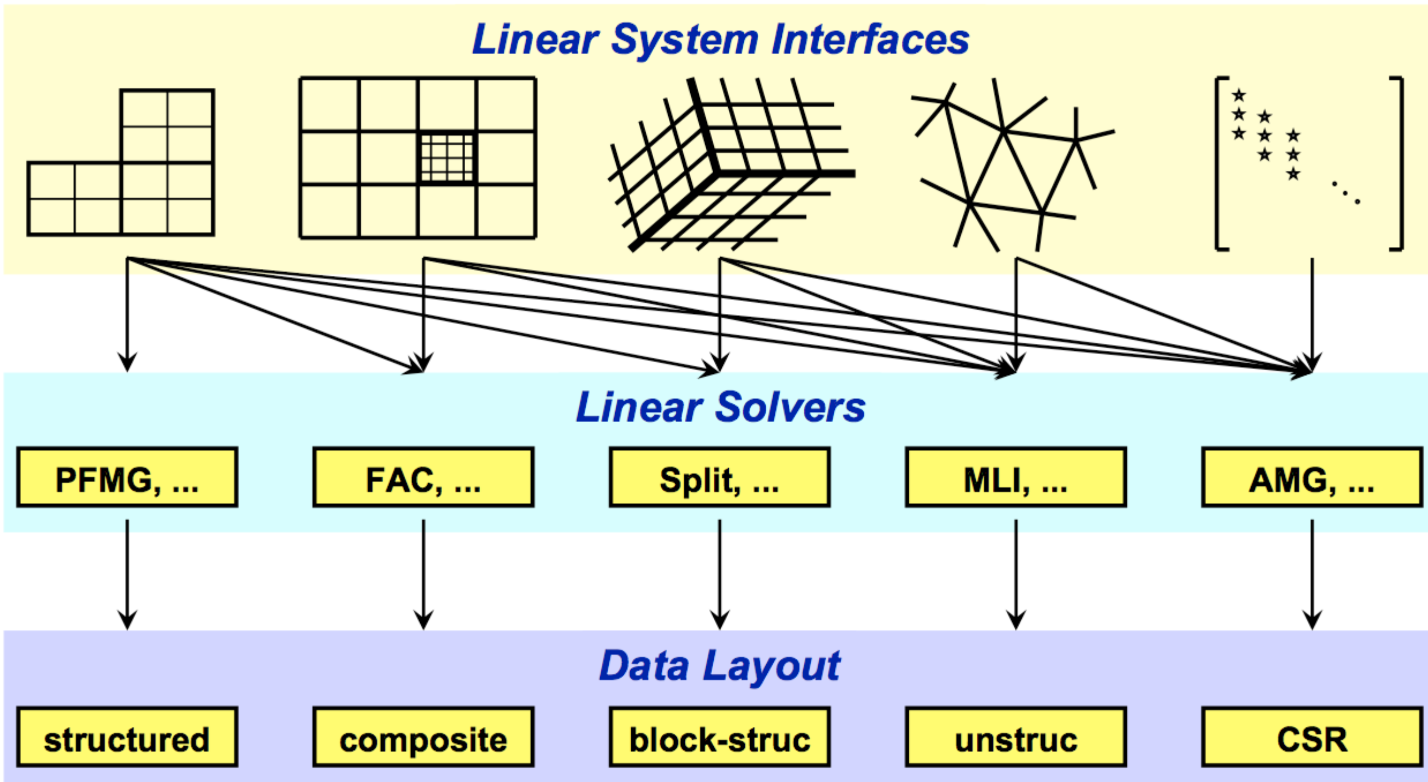
Trilinos Framework (Develop @ SNL)

Full Vertical Solver Coverage

Trilinos

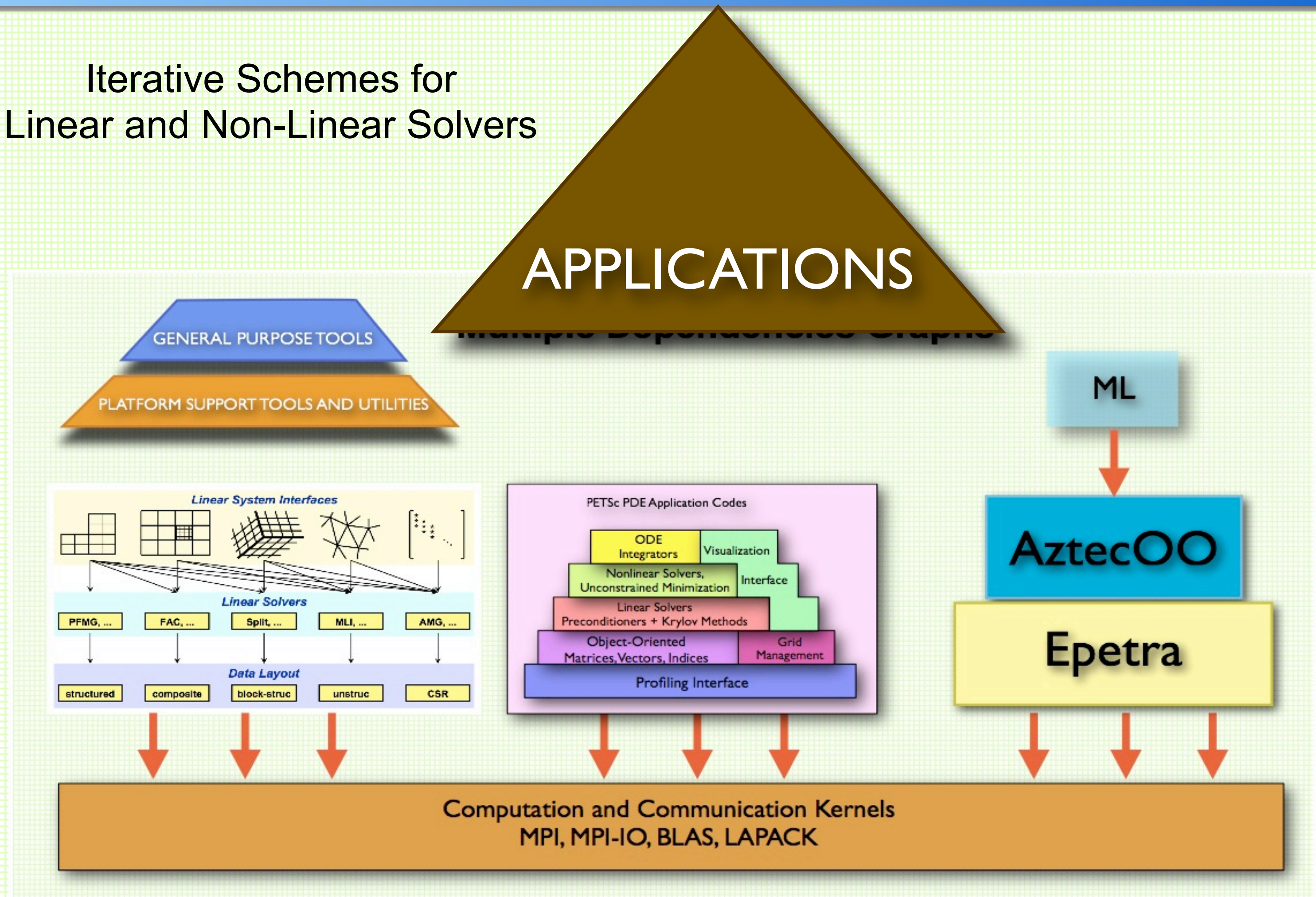
Optimization **Unconstrained:** **Constrained:**	Find $u \in \Re^n$ that minimizes $g(u)$ Find $x \in \Re^m$ and $u \in \Re^n$ that minimizes $g(x,u)$ s.t. $f(x,u)=0$	**Sensitivities (Automatic Differentiation: Sacado)**	**MOOCHO**
Bifurcation Analysis	Given nonlinear operator $F(x,u) \in \Re^{n+m}$ For $F(x,u)=0$ find space $u \in U \ni \frac{\partial F}{\partial x}$		**LOCA**
Transient Problems **DAEs/ODEs:**	Solve $f(\dot{x}(t), x(t), t) = 0$ $t \in [0,T], x(0)=x_0, \dot{x}(0)=x_0'$ for $x(t) \in \Re^n, t \in [0,T]$		**Rythmos**
Nonlinear Problems	Given nonlinear operator $F(x) \in \Re^m \rightarrow \Re$ Solve $F(x)=0 \quad x \in \Re^n$		**NOX**
Linear Problems **Linear Equations:** **Eigen Problems:**	Given Linear Ops (Matrices) $A, B \in \Re^{m \times n}$ Solve $Ax=b$ for $x \in \Re^n$ Solve $A\nu = \lambda B\nu$ for (all) $\nu \in \Re^n, \quad \lambda \in$		**AztecOO** **Belos** **Ifpack, ML, etc...** **Anasazi**
Distributed Linear Algebra **Matrix/Graph Equations:** **Vector Problems:**	Compute $y = Ax; A = A(G); A \in \Re^{m \times n}, G \in \Im^{m \times n}$ Compute $y = \alpha x + \beta w; \alpha = \langle x, y \rangle; x, y \in \Re^n$		**Epetra** **Tpetra**

Hypre (Develop @ LLNL)



Overlapping Functionality

Iterative Schemes for
Linear and Non-Linear Solvers



Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations *(cont..)* $Ax = b$ or $AX = B$	Iterative Methods	Conjugate Gradient	AztecOO (Trilinos) PETSc
		GMRES	AztecOO PETSc Hypre
		CG Squared	AztecOO PETSc
		Bi-CG Stab	AztecOO PETSc
		Quasi-Minimal Residual (QMR)	AztecOO
		Transpose Free QMR	AztecOO PETSc

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations (*cont..*) $Ax = b$ or $AX = B$	Iterative Methods (*cont..*)	SYMMLQ	PETSc
		Precondition CG	AztecOO PETSc Hypre
		Richardson	PETSc
		Block Jacobi Preconditioner	AztecOO PETSc Hypre
		Point Jocobi Preconditioner	AztecOO
		Least Squares Polynomials	PETSc

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations (*cont..*) $Ax = b$ or $AX = B$	Iterative Methods (*cont..*)	SOR Preconditioning	PETSc
		Overlapping Additive Schwartz	PETSc
		Approximate Inverse	Hypre
		Sparse LU preconditioner	AztecOO PETSc Hypre
		Incomplete LU (ILU) preconditioner	AztecOO
		Least Squares Polynomials	PETSc
	MultiGrid (MG) Methods	MG Preconditioner	PETSc Hypre
		Algebraic MG	Hypre
		Semi-coarsening	Hypre

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Linear Least Squares Problems	Least Squares	$min_x \|\| b - Ax \|\|_2$	ScaLAPACK
	Minimum Norm Solution	$min_x \|\| x \|\|_2$	ScaLAPACK
	Minimum Norm Least Squares	$min_x \|\| b - Ax \|\|_2$ $min_x \|\| x \|\|_2$	ScaLAPACK
Standard Eigenvalue Problem	Symmetric Eigenvalue Problem	$Az = \lambda z$ *For* $A=A^H$ or $A=A^T$	ScaLAPACK (dense) SLEPc (sparse)
Singular Value Problem	Singular Value Decomposition	$A = U\Sigma V^T$ $A = U\Sigma V^H$	ScaLAPACK (dense) SLEPc (sparse)
Generalized Symmetric Definite Eigenproblem	Eigenproblem	$Az = \lambda Bz$ $ABz = \lambda z$ $BAz = \lambda z$	ScaLAPACK (dense) SLEPc (sparse)

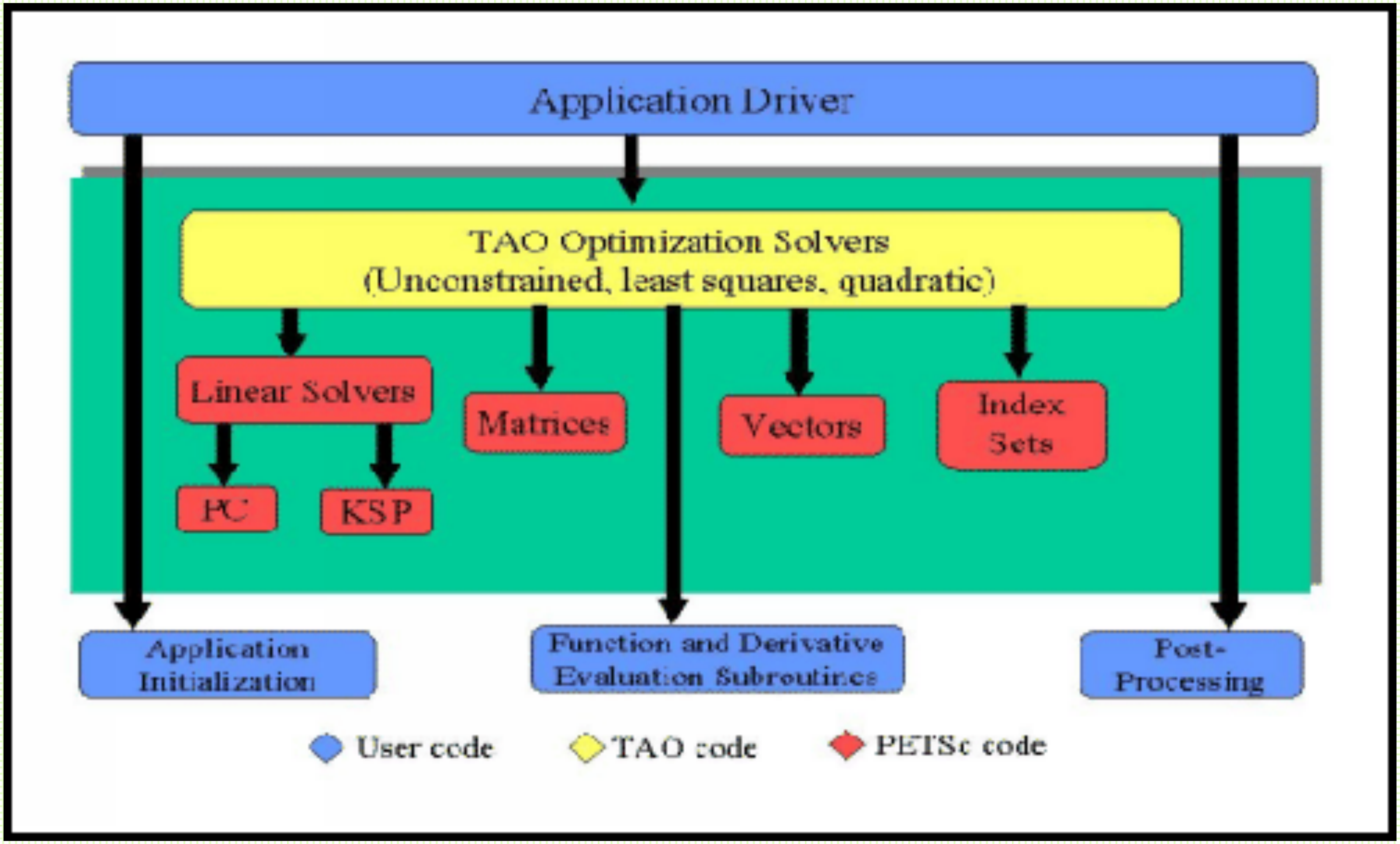
Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Non-Linear Equations $F(x) = 0,\ x \in R^n$ $F(X) \in R^m \rightarrow R^n$	Newton Based	Line Search	PETSc
		Trust Regions	PETSc
		Pseudo-Transient Continuation	PETSc
		Matrix Free	PETSc

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Non-Linear Optimization	Newton Based	Newton	TAO
		Finite-Difference Newton	TAO
		Quasi-Newton	TAO
		Non-linear Interior Point	TAO
	CG	Standard Non-linear CG	TAO
		Gradient Projections	TAO
	Semismoothing	Feasible Semismooth	TAO
		Unfeasible semismooth	TAO

TAO Interface Reusing PETSc



Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Ordinary Differential Equations	Integration	Adam-Moulton (Variable coefficient forms)	CVODE (SUNDIALS) CVODES
	Backward Differential Formula	Direct and Iterative Solvers	CVODE CVODES
Nonlinear Algebraic Equations	Inexact Newton	Line Search	KINSOL (SUNDIALS)
Differential Algebraic Equations	Backward Differential Formula	Direct and Iterative Solvers	IDA (SUNDIALS)

Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Techniques	Library
Writing Parallel Programs	Distributed Data Array (SPMD and MIMD)	Shared-Memory	Global Arrays
		Grid Generation	OVERTURE
		Structured Meshes	Hypre OVERTURE PETSc
		Semi-Structured Meshes	Hypre OVERTURE

Functionality in The DOE ACTS Collection

Computational Problem	Support	Technique	Library
Profiling	Algorithmic Performance	Automatic instrumentation	PETSc
		User Instrumentation	PETSc
	Execution Performance	Automatic Instrumentation	TAU
		User Instrumentation	TAU
Code Optimization	Library Installation	Linear Algebra Tuning	ATLAS

User Interfaces

```
CALL BLACS_GET( -1, 0, ICTXT )
 CALL BLACS_GRIDINIT( ICTXT, 'Row-major', NPROW, NPCOL )
:
 CALL BLACS_GRIDINFO( ICTXT, NPROW, NPCOL, MYROW, MYCOL )
:
:
 CALL PDGESV( N, NRHS, A, IA, JA, DESCA, IPIV, B, IB, JB, DESCB,
 $             INFO )
```

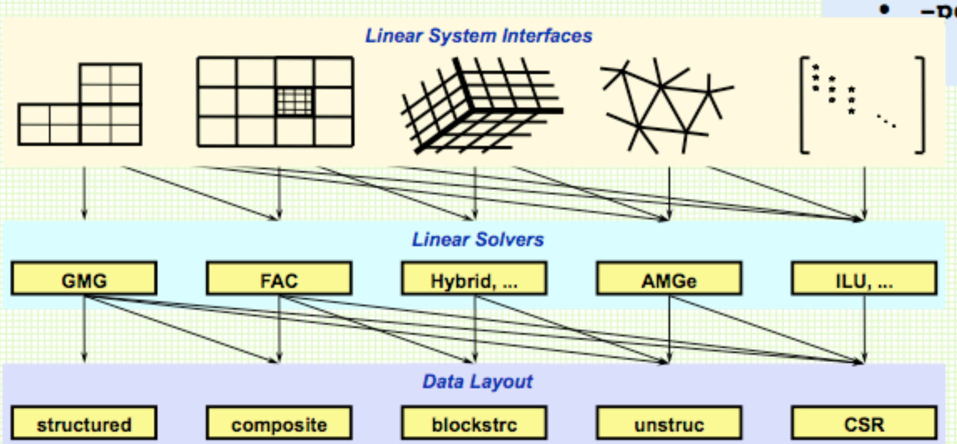
Library Calls

Command lines

- **-ksp_type [cg,gmres,bcgs,tfqmr, …]**
- **-pc_type [lu,ilu,jacobi,sor,asm, …]**

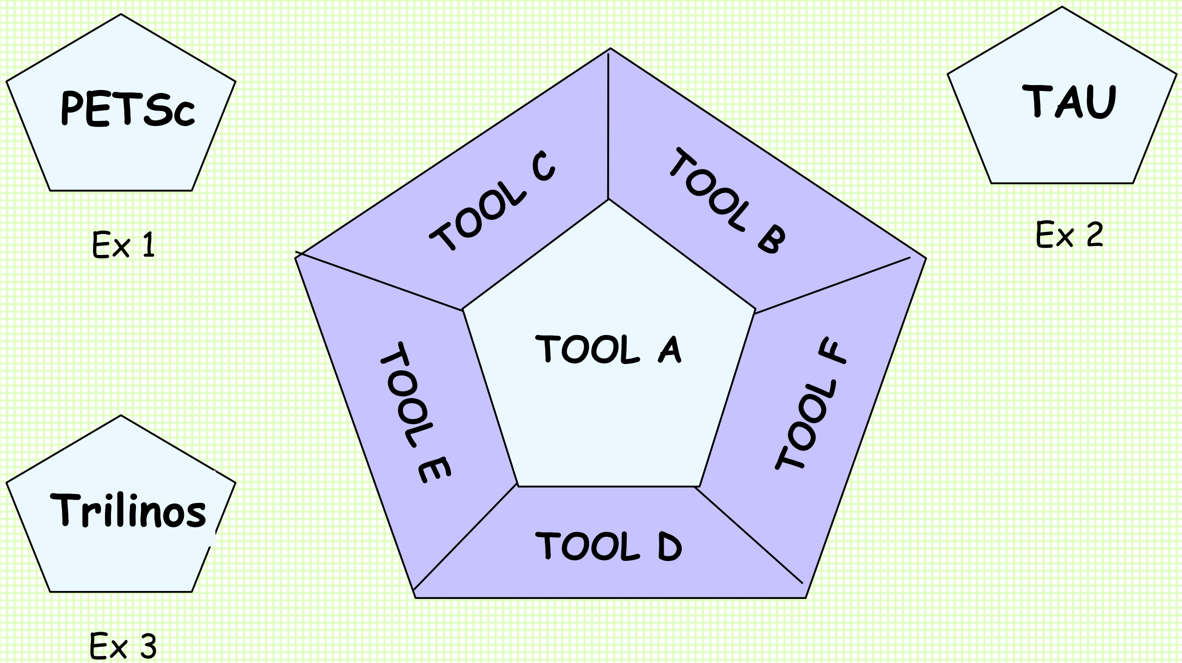
More advanced:

- **-ksp_max_it <max_iters>**
- **-ksp_gmres_restart <restart>**
- **-pc_asm_overlap <overlap>**



Problem Domain

Interoperability



PETSc Interoperability

Libraries/ Frameworks	Functionality
MUMPS	• Direct sparse linear solvers
SuperLU	• Direct sparse linear solvers
Trilinos	• ML • Epetra
Hypre	• Preconditioners
LAPACK/ ScaLAPACK	• Direct dense linear solver
⋮	

PETSc Interface

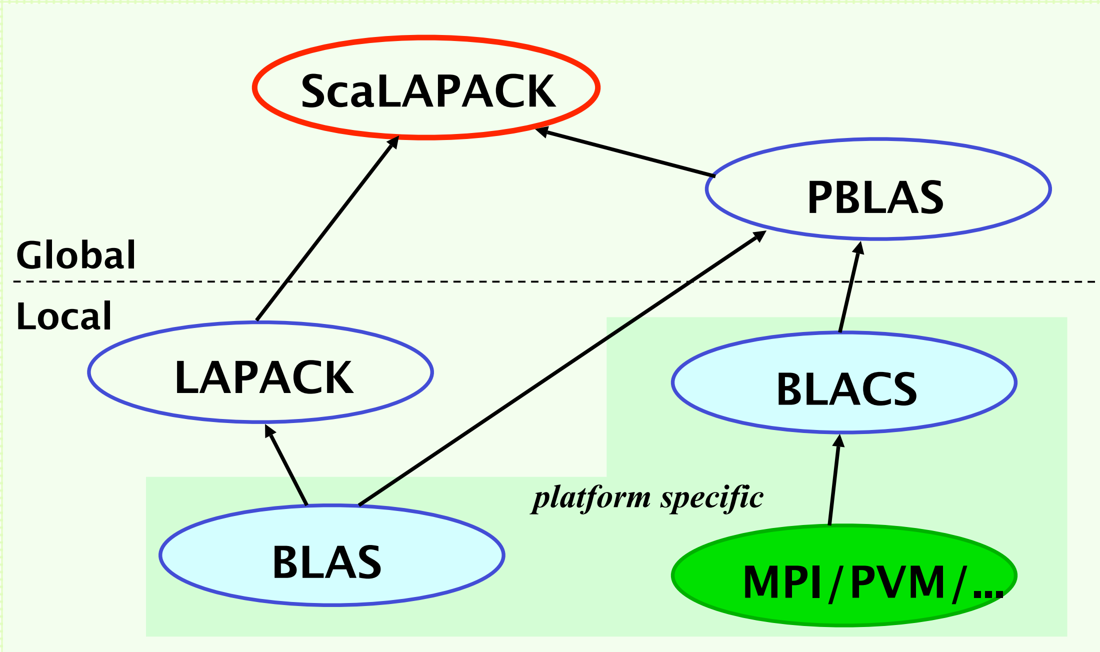
MatType	PCType	MatSolverPackage	Package (-pc_factor_mat_solver_package)
baij	cholesky	MAT_SOLVER_DSCPACK	dscpack
seqaij	lu	MAT_SOLVER_ESSL	essl
seqaij	lu	MAT_SOLVER_LUSOL	lusol
seqaij	lu	MAT_SOLVER_MATLAB	matlab
aij	lu	MAT_SOLVER_MUMPS	mumps
sbaij	cholesky		
plapack	lu	MAT_SOVLER_PLAPACK	plapack
plapack	cholesky		
aij	lu	MAT_SOLVER_SPOOLES	spooles
sbaij	cholesky		
seqaij	lu	MAT_SOLVER_SUPERLU	superlu
aij	lu	MAT_SOLVER_SUPERLU_DIST	superlu_dist
seqaij	lu	MAT_SOLVER_UMFPACK	umfpack

Table 5: Options for External Solvers

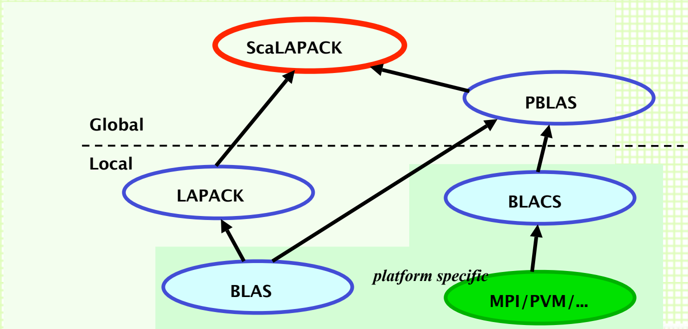
Trilinos interoperability

Library	Functionality
SuperLU	• Direct sparse linear solvers
MUMPS	• Direct sparse linear solvers
PETSc	• Epetra_PETSCAIJMatrix • ML accepts PETSc KSP for smoothers (fine grid only)
⋮	

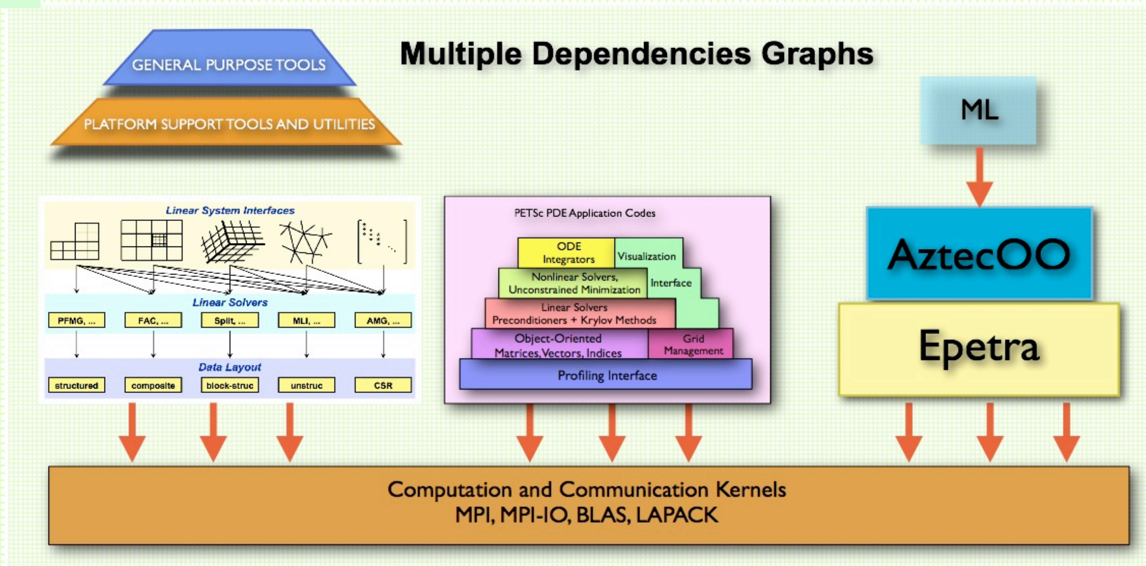
Installing and Building the Libraries



Software Dependency Graph



- Identify key common kernels
- Identify parameters that drive performance
- Profile and test (bottom-up)



Kernel Optimization

$Ax = b$ or $AX = B$

$Hx = b'$

$min_x \,||\, b - Ax \,||_2$

$min_x \,||\, x \,||_2$

$min_x \,||\, b - Ax \,||_2$

$min_x \,||\, x \,||_2$

$Az = \lambda z$

$A = U \Sigma V^T$

$A = U \Sigma V^H$

$Az = \lambda Bz$

$ABz = \lambda z$

$BAz = \lambda z$

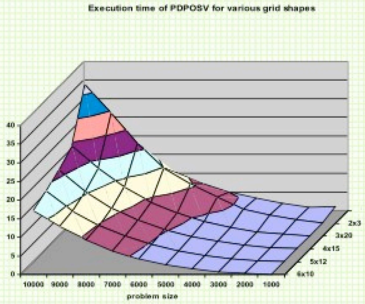
Auto-tuning

Exploit concurrency :
(in and out a node)
- Hybrid programming (MPI+threads)
- NUMA Aware operations

Kernel reusability:
- Bottom-Up automatic optimization
- Identify key parameters in the algorithm
- Run-time parameter control

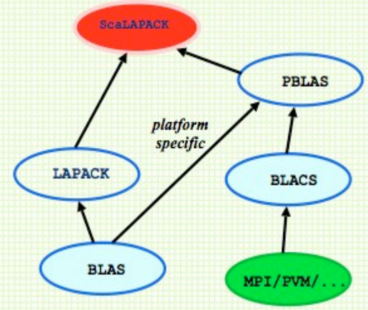
ACTS Software Sustainability Cycle

Profiling and Tracing Tools: TAU

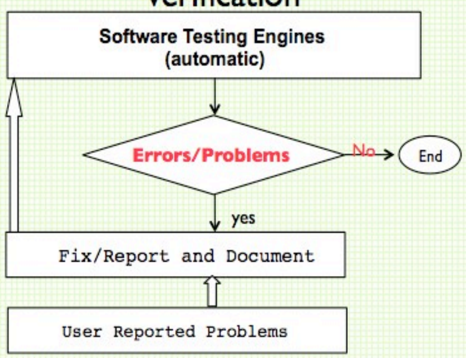


Performance and Scalability

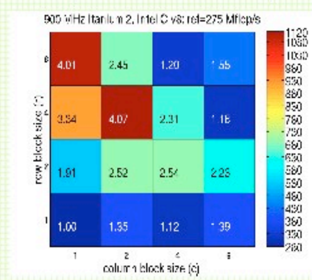
Software Dependency Graph



Automatic Testing and Verification



Auto-Tuning (OSKI, ATLAS,)



Summary

min[*time_to_first_solution*] (prototype)

min[*time_to_solution*] (production)

- Outlive Complexity
  - Increasingly sophisticated models
  - Model coupling
  - Interdisciplinary
- Sustained Performance
  - Increasingly complex algorithms
  - Increasingly diverse architectures
  - Increasingly demanding applications

(Software Evolution)

(Long-term deliverables)

min[*software-development-cost*]

max[*software_life*] and **max**[*resource_utilization*]

This Week at The Workshop

PROGRAM

Tuesday August 14	Wednesday August 15	Thursday August 16	Friday August 17
Registration from 7:45 AM	Doors open at 8:00 AM	Doors open at 8:00 AM	Doors open at 8:00 AM
Welcome Remarks and Introduction O. Marques T. Drummond 8:30 AM - 9:30 AM	***PETSc*** M. Knepley 8:30 AM - 10:30 AM	***Trilinos*** C. Siefert 8:30 AM - 10:30 AM	***SLEPc*** T. Drummond 8:30 AM - 9:30 AM
ScaLAPACK O. Marques 9:30 AM - 10:30 AM			***Zoltan*** E. Boman 9:30 AM - 10:30 AM
Break for Discussions 10:30 AM - 11:00 AM			

This Week at The Workshop

Tuesday August 14	Wednesday August 15	Thursday August 16	Friday August 17
Global Arrays B. Palmer 11:00 AM - 12:00 PM	***TAO*** J. Sarich 11:00 AM - 12:00 PM	***SuperLU*** O. Marques 11:00 AM - 12:00 PM	***HYPRE*** T. Kolev 11:00 AM - 12:30 PM
Working Lunch 12:00 PM - 1:00 PM			***Working Lunch*** 12:30 PM - 1:30 PM
TAU S. Shende 1:00 PM - 2:00 PM	***Invited Talk*** Katherine Yelick 1:00 PM - 2:00 PM	***Overture*** B. Henshaw 1:00 PM - 2:00 PM	***Visit*** C. Harrison H. Krishnan 1:30 PM - 2:30 PM
Break Sessions 2:00 PM - 2:15 PM			
Carver@NERSC H. Wasserman 2:05 PM – 2:15 PM			

This Week at The Workshop

TAU Hands-on S. Shende 2:15 PM - 3:30 PM	***SUNDIALS*** C. Woodward 2:15 PM - 3:30 PM	***Overture Hands-on*** B. Henshaw 2:15 PM - 3:30 PM	Break 2:30 PM - 2:40 PM ***VisIt Hands-on*** C. Harrison H. Krishnan 2:40 PM - 3:30 PM
ScaLAPACK Hands-on O. Marques 3:30 PM - 4:30 PM	***PETSc Hands-on*** M. Knepley 3:30 PM - 4:30 PM	***Trilinos Hands-on*** C. Siefert 3:30 PM - 4:30 PM	***Concluding Remarks*** **Workshop Adjourns**
Global Arrays Hands-on B. Palmer 4:30 PM - 5:30 PM	***TAO Hands-on*** J. Sarich 4:30 PM - 5:30 PM	***SuperLU Hands-on*** O. Marques 4:30 PM - 5:30 PM	
Working Dinner 7:00 PM - 9:30 PM			

ParaTools

The banquet dinner is sponsored in part by ParaTools

This Week at The Workshop

Two Accounts:

- NERSC Accounts (login to carver.nersc.gov)
  Please Return signed computer policy form

Misc.

- Special meals - See Yeen
- List of restaurants

Acknowledgements

- **National Energy Research Scientific Computing Center (NERSC)** for the use of their I Linux Cluster (magellan) - **Harvey Wasserman** from NERSC - USG

- **Katherine Day and Jan Hennessey** for all the great management and support running all the logistics of the workshop

- **To all the speakers and teams represented** at the 13th DOE ACTS Collection Workshop

- **DOE Office of Science** sponsors of this workshop

- **U of Oregon and ParaTools** for their support creating the ACTS Collection LiveDVDs and partially sponsoring the dinner tonight